Experimental and Molecular Dynamics Investigation of Interfacial Tension Between CO_2 and Brine Under High Temperature and Elevated Pressure Conditions

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We have investigated the dependence of interfacial tension (IFT) of (CO_2 + brine) on temperature, pressure and salinity (including both salt type and molality) over the range of conditions applicable to CO_2 storage in saline aquifers. Measurements have been made of the IFT between carbon dioxide and (NaCl + KCl)(aq), $CaCl_2$(aq), $MgCl_2$(aq) and Na_2SO_4(aq) with molalities from (0.49 to 5.0) mol·kg^{-1}. The measurement were made at temperatures between (298 and 448) K at various pressures up to 50 MPa. The pendant drop method was implemented in a high-pressure view cell filled with water-saturated CO_2. The drop to be imaged was created by injecting brine from a high-pressure syringe pump into a capillary sealed through the top of cell. The expanded uncertainties of the experiment at 95 % confidence are 0.05 K in temperature and 70 kPa in pressure. For the interfacial tension, the overall expanded relative uncertainty at 95 % confidence was 1.6%. Long time equilibrium molecular dynamics (MD) simulation were performed to study the interaction among water, ions and CO_2 on the interface. Both the experimental and simulation results show that interfacial tension increases linearly with molality. Furthermore, they also show that at constant temperature and pressure, the interfacial tension is the same function of the positive charge molality for all salts investigated in this work.